

# C-C And C-N Rotational Barriers In Vinyl Ketene And Vinyl Isocyanate

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## Summary

The conformational behavior and structural stability of vinyl ketene and vinyl isocyanate were investigated by utilizing ab initio calculations with 6-311 + + G\*\* basis set at the Density Functional (B3LYP) level. Both molecules were predicted to have the s-cis double left right arrow s-trans conformational equilibrium with the s-trans form being the predominant conformer for the two molecules. Full optimization was performed at the ground and transition states in the two molecules. The calculated rotational barriers in the systems were compared with each other and it was found that the barrier of the internal rotation around the C-C single bond in vinyl ketene was much higher than that of the corresponding C-N bond in the vinyl isocyanate. The vibrational frequencies were computed at the DFT-B3LYP level and the calculated infrared and Raman spectra of the cis-trans mixtures of the two molecules were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the molecules. (C) 2001 Elsevier Science B.V. All rights reserved.

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